ELSEVIER

Physica C 282–287 (1997) 1659–1660

PHYSICA C

Energy gap dispersion in bilayered cuprates

M.V.Eremin and I.A.Larionov

Faculty of Physics, Kazan State University, Kazan 420008, Russia

Using the singlet correlated band model the hole-phonon coupling constants with buckling oxygen modes have been calculated for $YBa_2Cu_3O_7$. The phonon mediated interaction enhances d-wave critical temperature, caused by superexhange interaction of copper spins.

1. INTRODUCTION

It is commonly believed that carrier holes in layered cuprates reside in the singlet correlated band [1,2]. Nevertheless, the problem of hole-phonons coupling is still far from being completely understood. In present paper we report part of our results concerning the coupling of the singlet correlated holes with so-called buckling modes. Recently, in [3] these modes were introduced for the explanation of the oxygen isotope effect in the cuprates and as a possible mechanism for the d-wave superconductivity.

2. PHONON COUPLING

In present calculations we follow the idea [4] and references therein. In YBaCuO compounds the holes distributed over the oxygen positions in the plane interact with the electric field perpendicular to the plane, which mainly comes from the yttrium ion. The Hamiltonian of perpendicular to the plane energy vibrations is given by

$$\mathrm{H}_{h-ph} = e\sum_{\mathbf{n}\sigma}\left\{\mathbf{E}_x\mathbf{u}_x\left(a\mathbf{n}+\frac{a\mathbf{x}}{2}\right)\mathbf{p}^{\sigma\sigma}_{\mathbf{n}\mathbf{x}} + \mathbf{E}_y\mathbf{u}_y\left(a\mathbf{n}+\frac{a\mathbf{y}}{2}\right)\mathbf{p}^{\sigma\sigma}_{\mathbf{n}\mathbf{y}}\right\} \qquad (1)$$

Here $\mathbf{p}^{\sigma\sigma}_{\mathbf{n}x}, \mathbf{p}^{\sigma\sigma}_{\mathbf{n}y}$ are Hubbard operators for the oxygen holes, $\mathbf{u}_x(\mathbf{n})$, $\mathbf{u}_y(\mathbf{n})$ are displacement vectors of O(2) and O(3) positions in the unit cell with number n, **x** and **y** are the unit vectors along the **a** and **b** axes, respectively, $\mathbf{E}_x$ and $\mathbf{E}_y$ are the electric field components along the **c** axis. Recently, in [5], these electric fields were calculated self-consistently. They are equal $\mathbf{E}_x=1.2\cdot10^8$ V/cm, $\mathbf{E}_y=1.5\cdot10^8$ V/cm. For simplicity below we assume $\mathbf{E}_x=\mathbf{E}_y=\mathbf{E}=1.35\cdot10^8$ V/cm because of the difference between them is relatively small.

Calculating the commutator $[\Psi^{\downarrow,pd}_{\mathbf{k}}, \mathrm{H}_{h-ph}]$ and using the equation

$$[\Psi^{\downarrow,pd}_{\mathbf{k}}, \mathrm{H}_{h-ph}] = \sum_{\alpha,\mathbf{q}} V^{\alpha}(q)\Psi^{\downarrow,pd}_{\mathbf{k}-\mathbf{q}}(b_{\mathbf{q}}+b^{+}_{-\mathbf{q}}) \qquad (2)$$

where $\Psi^{\downarrow,pd}_{\mathbf{k}}$ are the quasipartical operators of the singlet correlated oxygen holes [1,2], we have found

$$V^{\alpha}(\mathbf{q}) = \frac{e}{2}\mathbf{E}\sqrt{\frac{\hbar}{2m\omega_{\alpha}}}\left[\cos\left(\frac{q_x}{2}\right)\pm\cos\left(\frac{q_y}{2}\right)\right] \qquad (3)$$

Here $\omega_\alpha=\omega_{A1g}$, ω_{B1g}. Accord to [6] they are $\omega_{A1g}=440$ cm^{-1}, $\omega_{B1g}=340$ cm^{-1}. Because of the difference between ω_{A1g} and ω_{B1g} is not so important we have taken them equal to $\omega=400$cm^{-1}.

PII S0921-4534(97)00913-1